3,3,3-Trifluoro-2,2-bis(trifluoromethyl)propanoic acid

917951-63-4 | DTXSID00633413

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.07

Global applicability domain: Inside

Local applicability domain index: 3.57e-01

Confidence level: 6.87e-01

Nearest Neighbors from the Training Set

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Hexafluoroacetone
Measured: 1.46
Predicted: 1.55

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2-Methylpropyl diethylcarbamate
Measured: 2.82
Predicted: 2.75

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2-Ethylhexyl methacrylate
Measured: 4.54
Predicted: 4.39